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AB INITIO CALCULATIONS OF POINT DEFECTS IN SILICON ON MASSIVELY PARALLEL ENVIRONMENTS,

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Quantitative information, using theoretical first-principles approaches, about fundamental parameters of point defects in Si is critical to a microscopic understanding of diffusion processes during Si device processing. Among the first-principles approaches, density-functional theory (DFT) in the local-density approximation (LDA) and pseudopotential method have yielded accurate results for a wide range of materials. Furthermore, advances in numerical algorithms and in computational hardware, particularly the introduction of massively parallel-processing platforms, now makes feasible the *ab initio* treatment of technologically important materials.

To demonstrate these efforts, we will present a series of *ab initio* total-energy calculations of vacancies and self-interstitial defects in Si. The calculations were carried out on an Intel-Paragon, a TMC-CM5 and a Cray-T3D using various programming models. A supercell containing 32 to 216 Si atoms was used for the calculations to examine size effects.

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